A generic approach for live prediction of the risk of agricultural field runoff and delivery to watercourses: linking parsimonious soil-water-connectivity models with live weather data APIs in decision tools

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A generic approach for live prediction of the risk of agricultural field runoff and delivery to watercourses: linking parsimonious soil-water-connectivity models with live weather data APIs in decision tools

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Abstract

This paper describes the development and application of a novel and generic framework for parsimonious soil-water interaction models to predict the risk of agro-chemical runoff. The underpinning models represent two scales to predict runoff risk in fields and the delivery of mobilised pesticides to river channel networks. Parsimonious field and landscape scale runoff risk models were constructed using a number of pre-computed parameters in combination with live rainfall data. The precomputed parameters included spatially-distributed historical rainfall data to determine long term average soil water content and the sensitivity of land use and soil type combinations to runoff. These were combined with real-time live rainfall data, freely available through open data portals and APIs, to determine runoff risk using SCS Curve Numbers. The rainfall data was stored to provide antecedent, current and future rainfall inputs. For the landscape scale model, the delivery risk of mobilised pesticides to the river network included intrinsic landscape factors. The application of the framework is illustrated for two case studies at field and catchment scales, covering acid herbicide at field scale and metaldehyde at landscape scale. Web tools were developed and the outputs provide spatially and temporally explicit predictions of runoff and pesticide delivery risk at 1km^2 resolution. The model parsimony reflects the driving nature of rainfall and soil saturation for runoff risk and the critical influence of both surface and drain flow connectivity for the risk of mobilised pesticide being delivered to watercourses. The novelty of this research lies in the coupling of live spatially-distributed weather data with precomputed runoff and delivery risk parameters for crop and soil types and historical rainfall trends. The generic nature of the framework supports the ability to model the runoff and field-to-channel delivery risk associated with *any* in-field agricultural application assuming application rate data are available.

1. Introduction

Rainfall-induced surface and subsurface runoff mobilises and transports the chemicals used for in-field agricultural applications (fertilisers, herbicides and pesticides) from land to receiving freshwaters. Agriculture is therefore a significant source of water pollution, affecting drinking water quality and treatment costs. In England, for example, water companies spent £92 million in 2008-09 removing pollutants from water supplies to meet drinking water standards (National Audit Office, 2010). However, for some pollutants, such as metaldehyde, there are currently no cost-effective methods of removal, although the UK's first treatment plant has recently been constructed at significant cost to the water company in question[1]. Concentrations of such agrochemicals above safe limits in surface and groundwaters creates not only environmental risk, but also a risk to human health.

Agricultural applications can enter surface water via a number of pathways. Spills, spray-drift and illegal disposal are generally managed by best practice guidance and prosecution. Surface and subsurface runoff can transport agrochemicals in dissolved and particulate form, from the field to watercourses. The proportion that is removed in solution relative to that attached to mobilised soil particles depends on the intrinsic soil properties, topography / slope and the characteristics of the agrochemicals such as pesticides, including their sorption and solubility properties (Louchart et al., 2001; Guo et al., 2004; Vinten et al., 2005; Kay et al., 2009; Newell-Price et al., 2011).

The biggest driver of surface and subsurface runoff is precipitation and the timing and characteristics of the first rainfall event after application are very important. Antecedent weather determines the wetness of the soil and therefore the degree to which the chemical is 'held' by the soil. Applications made to wet soil (at field capacity or wetter), or just before heavy rainfall, are more likely to be lost in surface runoff or by-pass flow to field drains, with negative environmental and water quality impacts as they are transferred to surface or groundwater (Mitchell et al., 2005; Gao et al., 2008; Lapworth et al., 2012), although the propensity for mobilised pollution to reach watercourses also depends on additional factors affecting delivery (e.g. the status and maintenance of field drains, the topology of the landscape, distance to watercourses). Thus, water pollution risk is enhanced by poor timing of applications in relation to weather events which can result in pollutant concentrations in surface waters that exceed drinking water standards (Petty et al., 2003).

In addition to the environmental benefits, the efficacy of any agricultural application is severely reduced if runoff washes it from the crop or the field. For the farmer, the reduced efficacy leads to risks of reduced yields (income) and/or increased costs (and thereby lower gross margins) if the treatment has to be re-applied to protect the crop. The annual cost to farmers of agricultural runoff has been estimated at £238m (Jacobs UK Ltd, 2008) a significant part of which can be attributed to the impact of runoff losses associated with compromised pesticide and herbicide effectiveness. There are additional environmental (damage) costs and, in future, there may be financial penalties for pesticides and herbicides being washed into watercourses. Preventing agro-chemicals reaching surface and groundwaters by imparting source control measures is more cost-effective than water treatment and some initial research has identified a benefit-to-cost ratio of 65:1 for prevention over treatment (Defra, 2013).

[1] https://wwtonline.co.uk/features/project-focus-hall-claims-uk-first-in-water-treatment

Direct detection of the source of pesticides and herbicides carried by runoff is difficult due to the diffuse nature and temporal variability of the sources and the high cost of instrumentation (Meyer et al., 2019) and with some pollutants, the length of time taken to analyse water samples makes real-time risk mapping impractical. Consequently, modelling water pollution risk is the only practical option in most cases.

This paper describes the development of two decision tools operating over different scales of decision making. The tools provide interfaces to two parsimonious soil-water runoff models; one supporting on-farm decisions at the field scale and another supporting landscape scale management. Both include inputs and outputs at a1km^2 spatial scale, but their aims are very different and their outputs should be interpreted in very different ways. The field scale tool provides the end-user with point-based information of runoff risk derived from a model operating over each 1km^2 independently. It uses a meta-model to forecast surface runoff risk for a given land use on a given soil from recent recorded and forecast rainfall alone. It aims to support farmers and land managers to better manage pesticide applications. The catchment scale model also uses a 1km^2 scale (in part because most of the data available to support such analyses and models are at best at 1 km^2 resolution). However, the inputs and outputs do not describe processes that operate independently over each 1km^2. Rather, the inputs describe landscape processes that are topologically connected such as field drain and surface flows as well as landscape connectivity between fields and watercourses. In this case, the outputs provide Tier 1 screening to identify hotspots requiring further investigation, with the aim of supporting informed on-the-ground catchment management by environmental agencies and water companies.

2. Background

This research is informed by two limitations arising from previous work: the difficulties of determining antecedent soil water status (and thereby the potential for soil to hold water) and the temporally static nature of many landscape scale decision support tools in this domain.

2.1 Modelling Runoff

The SCS Curve Number (CN) method (USDA SCS, 1972) is commonly used to model surface runoff depth from rainfall amount, soil surface characteristics and antecedent wetness. It is also used to predict runoff and infiltration (USDA, 2004). It is applicable to small catchments (≤ 6,500 ha) (NRCS, 2002) and has been implemented in models to estimate agrochemical transport to water (e.g. CREAMS - Knisel 1980; SWAT - Arnold *et al*., 1998; PRZM - Carsel et al., 1998; APEX - Williams and Izaurralde, 2006) and has been shown to be robust for a range of climates, soil types and land uses (e.g. Gassman et al., 2007). It has been found to perform better than an infiltration model in modelling runoff in an agricultural catchment in England (Kannan et al., 2007). Many CN models predict runoff depths for individual weather events using an empirical relationship between direct runoff depth, rainfall amount, soil surface characteristics and antecedent wetness (USDA, 2004). The rainfall amount at which runoff starts depends on the maximum potential retention, which in turn, depends on land use and soil type. The CN approach provides a widely used and effective method for estimating direct runoff due to rainfall. Despite its simplicity, and the availability of CNs for various land use and soil type combinations (USDA, 2004; Chow et al., 1988; Pilgrim & Cordery, 1993), operationally it can be difficult to estimate the antecedent soil moisture conditions. Although the antecedent soil water status has been estimated from 5-day antecedent rainfall (e.g. Mishra *et al*., 2005), this has been shown to be poorly correlated with maximum potential retention (USDA, 2004).

2.2 Decision Support Tools

User-facing decision tools started to emerge with the advent of easily programmable GISs with graphical user interfaces. These were developed to support farming compliance under newly legislated environmental directives, such as the Water Framework Directive (WFD, 2000) in Europe, and sought to minimise the externalities of agricultural activity on waterbodies. Decision tools, for use by both farmers and policy makers, were developed over a range of spatial scales: nationally, at typical scales of 1, 5 and 10 km^2 and Europe-wide at scales of 10, 20 and 50 km^2. Examples of UK models include those of Webb and Misselbrook (2004), Chadwick et al. (2005), Chambers et al. (1999), Davison et al. (2008), Lord and Anthony (2000) and Lord (1992) many of which are summarised in Anthony et al. (2008). At the European scale, similar models include PyCatch (Schmitz et al., 2017) and the FOOTPRINT (Functional Tools for Pesticide Risk Assessment and Management) framework which integrates pesticide use information with a physically based field scale soil water model (Jarvis et al., 2000) for drainage and leaching pathways and PRZM (Suarez, 2005) for runoff and erosion pathways. Hydrological modelling frameworks have also been used to simulate agrochemical runoff (Kannan et al., 2006; Ficklin et al., 2013; Bannwarth et al., 2013; Zhang et al., 2018). A key and unavoidable characteristic of existing landscape process-based models is that their outputs and the scales they report over are spatially and temporally incompatible with the expectations and needs of land managers. Here, a key limitation is the fact they are underpinned by highly static, spatially and temporally aggregated data by way of model inputs such as underlying soil types, drainage, land use, climate, terrain characteristics and farming practice.

2.3 Research aims

The critical gap, common to SCN models and decision support tools, regardless of scale, is that they do not incorporate live and dynamically updated data on soil condition or rainfall. Very detailed and precise prediction models for soil water balances and associated runoff, leaching and pollution risks (e.g. Morselli et al., 2018; Pullan et al., 2016) require specific, local information that cannot be obtained from generalised GIS layers, often requiring in situ parameterisation and measurement. This is because data may not be freely available (e.g. soils data), are dis-aggregates of coarser scale data (e.g. agricultural land use) or are themselves modelled outputs (e.g. landscape connectivity data). A further key issue across scales and model types is that they commonly suffer from poor performance when evaluated using monitoring data despite being very heavily parameterised (Kim et al., 2010; Bieger et al., 2014; Gassman et al., 2014; Zeiger and Hubbart, 2016). For this reason, recent research has explored the use of parsimonious tools for pesticide risk (e.g. Gassman et al., 2013; Steffens et al., 2015; Pullan et al., 2016).

It is against this background, that this paper describes the development of two decision tools providing real-time, spatially-explicit and temporally-dynamic field runoff and field-to-channel pesticide delivery risk information for supporting decisions regarding pesticide application (field scale) or management of surface water withdrawal for public water supply (catchment scale). These are demonstrated for two example agro-chemical applications in two differing environmental settings in the UK. The tools incorporate parsimonious field runoff and field-to-channel delivery models that combine real-time data of antecedent, current and predicted rainfall obtained from a national meteorological institute API. Both tools generate real-time predictions of current and future agro-chemical field runoff or field-to-channel delivery risk over a 5-day window. A key distinction is that the field scale tool has a focus on quantifying runoff risk, whereas the catchment scale tool focuses on quantifying the risk of delivery to the channel network – i.e. pesticide delivery risk rather than runoff risk.

3. Methods and new models

Two case-study catchments were selected. The Wissey catchment in eastern England is dominated by arable cropping and has a potential risk of metaldehyde in waterbodies. Metaldehyde is used to treat slugs on oil seed rape, potatoes and horticultural crops and was responsible for 23% of failures to meet drinking water standards in the 4th quarter of 2016 in England and Wales (Defra, 2017a). Metaldehyde also topped the list of pesticides which breached the 0.1 μg/l drinking water safety limit between 2013 and 2015 (Defra, 2017b). In contrast, the Teifi catchment in mid-Wales, is dominated by grassland used for livestock. Here, acid herbicide applications for managing weeds in pastures represents a risk for drinking water quality. Field and landscape (catchment) scale models were developed for both case studies using the methods described below. For illustration in this paper, the results present the application of the field model and tool for runoff risk in the Teifi catchment in Wales, and the landscape scale model and tool for metaldehyde delivery risk in the Wissey catchment in England.

3.1 Field scale model

3.1.1 Overview

The aim of the field scale model was to provide location specific information of current and predicted future (5 day) runoff risks, at a 1 km^2 grid cell scale representing the field. It sought to support on-farm decisions about agro-chemical applications and to provide forecasts of whether any surface runoff is expected at the field scale. Although a soil water balance model could be used to antecedent soil water conditions and the CN method (USDA, 2004) to assess potential field runoff in real-time, data and computational requirements are an important limitation. In addition, fully parameterised soil water balance models require a known starting condition and are prone to cumulative errors, particularly during periods of low rainfall. From an operation point of view, using a soil water balance model to estimate antecedent soil water conditions also requires the user (farmer) to collect and process rainfall data even during periods when runoff risk forecasts are not required. To overcome this, a meta-modelling approach was used to estimate antecedent soil conditions from soil type, long-term average soil water content for the day of year, recent recorded rainfall and short-term forecast rainfall. An overview of the field scale model is shown in Figure 1.

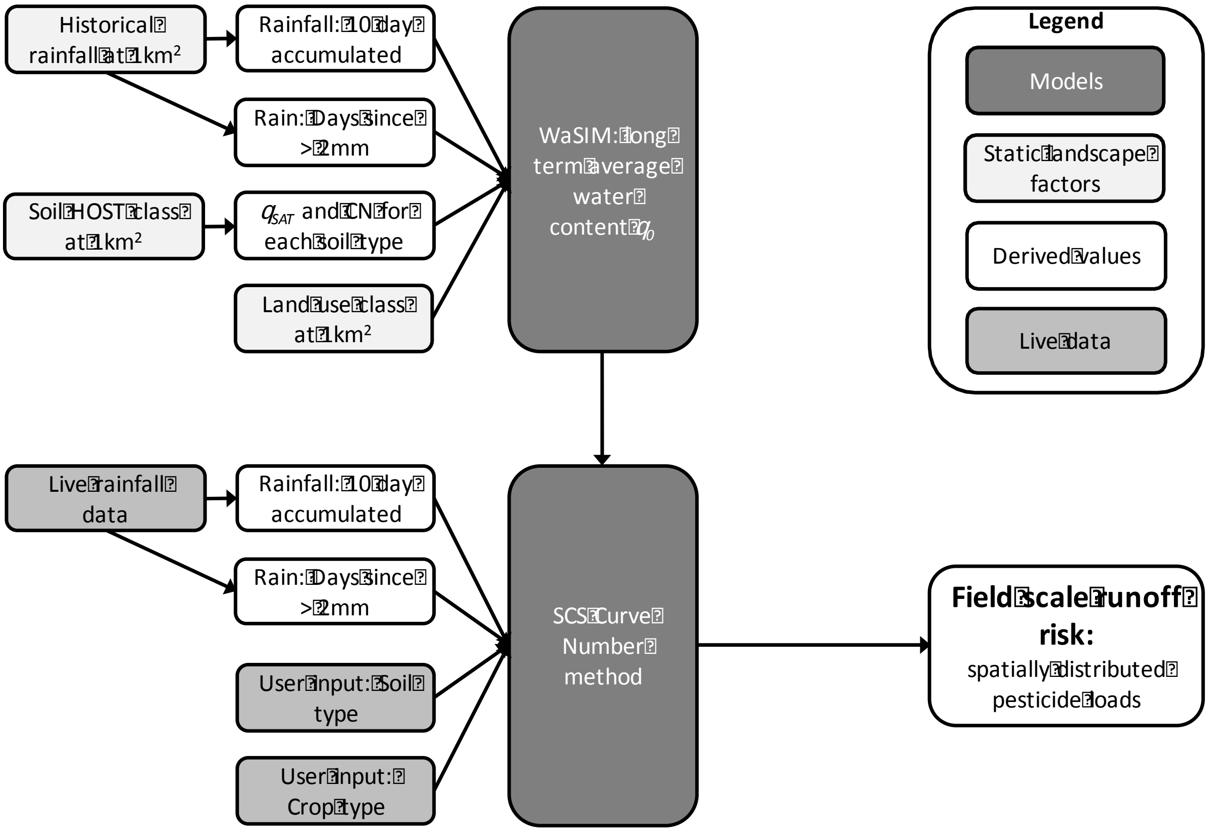

Figure 1. The field scale runoff risk model.

3.1.2 Data and Model

The soil water balance model, WaSim (Hess and Counsell, 2000), was used to estimate daily soil water condition (θ) using the approach described by Hess et al. (2010) and Holman et al. (2011). It used a long time-series (1961 to 2015) of daily rainfall and reference evapotranspiration data at 1 km^2 resolution from the CEH CHESS dataset (Robinson et al, 2016, 2017) for each of the 28 hydrology of soil type (HOST) (Boorman et al., 1995) classes found in England and Wales, and three land cover classes.

WaSim is a daily soil water balance model that simulates changes in root zone soil water content and water table position in response to weather and water management. It estimates changes in soil water content by combining data on rainfall, crop specific evapotranspiration, soil characteristics and field drainage. It estimates daily surface runoff using a CN approach based on the soil water content using the approach of Hawkins *et al*. (1985) and Garen (1996).

The water content of the upper (0 – 0.15 m) layer (θ_0) is estimated from daily effective rainfall, evapotranspiration and drainage to a lower layer. The proportion of the soil water stored above field capacity (θ_{FC}) that is released from a saturated soil increases from zero at θ_{FC} to a maximum at saturation (θ_{SAT}) following an exponential function (Raes and van Aelst, 1985) dependent on the texture of the upper soil layer. Validation of predicted field-scale runoff is difficult due to the paucity of field-scale runoff data for a sufficient range of soil, crop and climate conditions for national application. However, Holman et al. (2011) evaluated partitioning of hydrologically effective rainfall between slow and quick flow-paths in the WaSim model by upscaling to the catchment scale across all of England and Wales. For 27 out of the 29 HOST soil classes (Boorman et al., 1995) (peat soils excepted). The WaSim estimates of baseflow index (BFI) were within the 95% confidence intervals of the national-average BFI , suggesting that the model is adequately capturing the effect of soil type and wetness on runoff generation.

Using linear regression on a subset of the data (1961 – 2000), the daily soil water condition was modelled from the 10 previous days' accumulated rainfall (P_{10}), the number of days since the last day with rainfall >2 mm (P_2) and long-term average modelled daily soil water condition ($\overline{\theta_i}$) for each the day of the year, *i*. The resulting linear regression models were shown to fit well to the soil water conditions modelled by the soil water balance model for an independent timeseries (2001-2015), summarised in Section 3.1.3 and as described in Comber et al (2018). The parameterised regression model was then used with recent and short-term forecast rainfall data to forecast runoff, *R*, using the CN method of Hawkins *et al*. (1985) and Garen (1996) as follows: for rainfall, *P* (mm d^{-1}), greater than a threshold value, *I* (mm), direct runoff, *R* (mm d^{-1}), is estimated from:

$$R = \frac{(P-\lambda S)^2}{(P+(1-\lambda)S)} \text{ for } P > \lambda S \qquad (1)$$

$$R = 0 \text{ for } P \leq \lambda S$$

where *S* is the maximum retention, mm and the threshold *I* is defined as

$$I = \lambda S \qquad (2)$$

Note that λ (dimensionless) is an empirical value that represents the proportion of rainfall on a soil at average antecedent conditions that can fall without generating runoff, and is typically set to 0.2.

On a particular day, *S* was estimated from the retention at dry antecedent conditions, S_1 (mm), the relative saturation of the top 0.15 m of the soil, f_s (dimensionless) and two weighting factors, W_1 and W_2 for retention (Hawkins *et al*., 1985):

$$S = S_1\left[1 - \frac{f_s}{f_s + exp(W_1 - W_2 f_s)}\right] \qquad (3)$$

$$f_s = \frac{\theta_i}{\theta_s} \qquad (4)$$

$$W_1 = ln\left[\frac{1}{1 - \frac{S_3}{S_1}} - 1\right] + W_2 \qquad (5)$$

$$W_2 = 2\left[ln\left(\frac{0.5}{1-\frac{S_2}{S_1}} - 0.5\right) - ln\left(\frac{1}{1-\frac{S_3}{S_1}} - 1\right)\right] \quad (6)$$

The retention, S_n (mm), at dry (n = 1), average (n = 2) and wet (n=3) antecedent conditions, is estimated from the curve number, N_2 (dimensionless) at average antecedent conditions (Garen, 1996).

$$S_n = 250\left(\frac{100}{N_n} - 1\right) \quad (7)$$

$$N_1 = \frac{N_2}{2.281 - 0.01281N_2} \quad (8)$$

$$N_3 = \frac{N_2}{0.427 + 0.00573N_2} \quad (9)$$

3.1.3 Model Validation

Hess et al. (2010) used a continuous water balance model, WaSim (Hess and Counsell, 2000) to model daily soil water content and estimate daily surface runoff using a CN approach. WaSim is a one-dimensional, field-scale layered soil-water balance model that operates on a daily timestep. The water content of the upper (0 – 0.15 m) layer, θ_0 (dimensionless), is estimated from daily effective rainfall (P - R), evapotranspiration, E (mm d^{-1}) and drainage to a lower layer, D (mm d^{-1}). D increases with θ_0 from zero at field capacity, θ_{FC}, to a maximum at saturation, θ_{SAT}, following an exponential function (Raes and van Aelst, 1985):

$$D = \tau(\theta_0 - \theta_{FC})\frac{e^{(\theta_0-\theta_{FC})} - 1}{e^{(\theta_{SAT}-\theta_{FC})} - 1}150 \quad (10)$$

Where τ (d^{-1}) is the proportion of the soil water stored above field capacity that is released from a saturated soil in one day and is dependent on the soil texture, and 150 (mm) is the thickness of the upper soil layer.

Three linear regression models, M1 to M3, were calibrated against θ_0 for each soil and climate combination in each of the two study areas:

- M1 is a simple linear regression of θ_0 against the 5-day accumulated antecedent rainfall, P_5 under the expectation that for a given location and soil type, θ_0 will be correlated with the antecedent rainfall;
- M2 considered the 10-day accumulated antecedent rainfall, P_{10}, and the number of days since the last rainfall >2 mm, $J_{P>2}$;
- M3 considered the 10-day accumulated antecedent rainfall, P_{10}, the number of days since the last rainfall >2 mm, $J_{P>2}$ and also considers the long-term average value of θ_0 for the day of the year, ($\overline{\theta_i}$). This assumed that the effect of antecedent rainfall on θ_0 may vary with seasonal variation in θ_0. For example, a small P_{10} on at a time of year when the soil is generally wet would result in wetter antecedent conditions than at a time when the soil is generally drier.

Each model is summarised in Table 1 and was calibrated against the WaSim continuous model and then used to estimate θ_0.

Model Coefficients	Model 1 (M1)	Model 2 (M2)	Model 3 (M3)
X_1	Accumulated 5-day antecedent rainfall, P_5	Accumulated 10-day antecedent rainfall, P_{10}	Accumulated 10-day antecedent rainfall, P_{10}
X_2		Number of days since the last rainfall >2 mm, $J_{P>2}$	Number of days since the last rainfall >2 mm, $J_{P>2}$
X_3			Long-term average value of θ_0 for the day of the year, ($\overline{\theta_i}$)

Table 1. A summary of the different models that were evaluated.

Table 2 shows the coefficient estimates of the three locally calibrated linear models to estimate antecedent soil moisture conditions, adjusted for each site and soil type. It also includes the root mean squared error (RMSE), mm d^{-1}, between upper layer soil water content from a continuous model and the three meta-models for the calibration (1961-2000) and validation (2001-2015) periods. For the two models relying only on antecedent rainfall (M1 and M2) the intercept is the most important coefficient of the model, taking values close to the volume water fraction at field capacity. The M3 coefficients demonstrate the importance of including average soil moisture conditions and the major difference between parameters is driven by weather conditions rather than by soil type. Similarly the validation results show that M3 achieves the best results for both soil types and both climates. Moreover, the results suggest that introducing the daily average soil moisture content has an important impact on the quality of the model.

			Coefficients				RMSE	
Case Study	**Soil Type**	**Model**	**Intercept**	**X_1**	**X_2**	**X_3**	**Calibration**	**Validation**
Teifi	Clay Loam	M1	0.376	0.002			0.030	0.031
		M2	0.393	0.001	-0.004		0.027	0.029
		M3	0.126	0.001	-0.004	0.675	0.024	0.025
	Sandy Loam	M1	0.266	0.002			0.033	0.033
		M2	0.284	0.001	-0.004		0.030	0.031
		M3	0.090	0.001	-0.004	0.664	0.026	0.026
Wissey	Clay Loam	M1	0.351	0.003			0.035	0.032
		M2	0.361	0.002	-0.002		0.031	0.028
		M3	0.029	0.002	-0.002	0.875	0.023	0.020
	Sandy Loam	M1	0.241	0.004			0.033	0.033
		M2	0.252	0.002	-0.003		0.030	0.031
		M3	0.027	0.002	-0.002	0.833	0.026	0.026

Table 2. Coefficients of the three linear models and the root mean squared error (RMSE), mm d^{-1}, for the calibration (1961-2000) and validation (2001-2015) periods.

3.2 Landscape scale model

3.2.1 Overview

The landscape scale model provides spatially distributed information on pesticide delivery risk. The overarching aim was to identify field-to-channel delivery risk hotspots to support and inform catchment management and on-the-ground follow up by environmental agencies and water companies. It therefore identifies locations of high risk that may require further investigation. The landscape scale tool generates a spatially-distributed field-to-channel delivery risk surface to inform drinking water abstraction decisions. The output predicts the spatial pattern of mobilised pesticide loadings delivered to receiving watercourses. The parsimonious approach combines layers of intrinsic landscape scale factors, runoff and pollutant transfer, national historical daily rainfall data from the CEH Gridded Estimates of Areal Rainfall dataset (Keller et al., 2015), as well as live data of current and antecedent rainfall, as summarised in Figure 2.

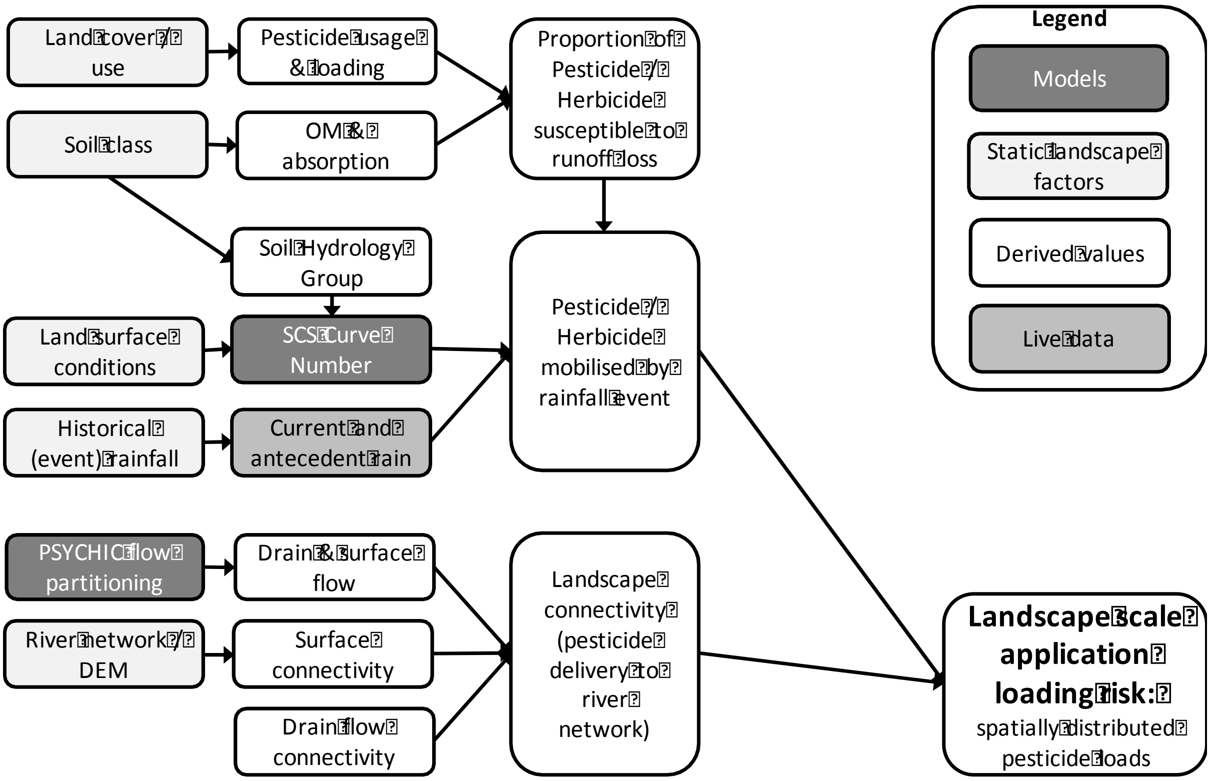

Figure 2. The parsimonious landscape scale model. OM = organic matter.

A source-mobilisation-delivery-impact model of the water pollutant transfer continuum (Lemunyon and Gilbert, 1993; Haygarth et al., 2005; Zhang et al., 2017) was adopted. In this framework, runoff following rainfall is the key mobilisation force and the proportion of pesticide load available for mobilisation into the runoff moving down the soil profile to field drains or downslope across the land surface is assumed to be the same as the ratio of runoff amount to event rainfall total. Pesticides are therefore partly absorbed by the soil and non-binding pesticides are mobilised in runoff. This multiplicative correction approach is similar to that used by Verro et al. (2002). The landscape model recognises that rainfall can reach watercourses via different delivery pathways (e.g. surface runoff, drain flow) and measures of hydrological connectivity between agricultural fields and the river channel network influence the propensity for mobilised pollution (e.g. pesticides) to reach the watercourses. In the case of the latter, surface runoff connectivity is calculated using distance to river channel and the downslope average slope gradient using a high resolution digital elevation model (DEM) and channel network data layer (Prosser and Rustomji, 2000; Walling and Zhang, 2004), whereas drain flow connectivity uses farm-type specific estimates based on recent surveys of drain maintenance associated with the upkeep of the permeable backfill or drain freeboard, as well as the frequency of supportive mole ploughing (Zhang et al., 2016).

3.2.2 Data and model

Data at 1 km^2 resolution were assembled for each case study area. The proportions of different land use including crop types in each grid cell (Comber et al., 2008) were matched with freely available data on pesticide application rates to determine pesticide loadings to farmed land. The land use data described in Comber (2008) uses advanced spatial disaggregation methods to robustly allocate agricultural census data from the June Survey of Agriculture and Horticulture (JAS). JAS data are reported at coarse spatial units (such as Parish level) and the disaggregation is to finer spatial units such as $1km^2$. This data underpins many tools supporting national level policy support. Garthwaite et al (2013; 2014; 2015) describe pesticide usage on different agricultural land uses and spatially distributed pesticide loadings to agricultural land were estimated by linking the land use proportions of each $1km^2$ to the reported pesticide usage for that land use.

The loadings from all applications to agricultural land are then modified to estimate the loading susceptible to runoff mobilisation and delivery from field-to-channel by the soil sorption capacity for the pesticide in question, which is modelled as a function of known pesticide behaviour and soil organic carbon content (% *OC*). Accordingly, the proportion of chemical loading susceptible to mobilisation and runoff loss with rainfall, *K* is calculated as follows:

$$K = \frac{1}{1 + Koc \times OC/100} \quad (11)$$

where *Koc* is a measure of the tendency of a chemical to bind to soils (an adsorption coefficient) set at 67 in the Wissey and 20 in the Teifi study catchments..

Runoff was estimated using the Mishra-Singh model (Mishra et al., 2005), a modified CN method, that accounts for event rainfall and antecedent soil moisture conditions. To estimate runoff (*R*, mm), event rainfall *(P*, mm) and the antecedent 5-day rainfall (P_5, mm) are required, as well as an estimate of storage depth (*S*, mm), initial abstraction (*Ia*) and an intermediary term, *M*:

$$S = \frac{25400}{CN} - 254 \quad (12)$$

$$Ia = \lambda S \quad (13)$$

$$M = -\left(\frac{(1+\lambda)}{2}\right)S + \sqrt{(1-\lambda)^2 S^2 4 P_5 S} \quad (14)$$

$$R = \left(\frac{(P - Ia)(P - Ia + M}{P - Ia + M + S}\right) \quad (15)$$

where λ is an empirical value which typically set to 0.2. The CN values for different soil types, land use and surface conditions are based on Hess et al. (2010) using the UK Hydrology of Soil Type (HOST) classification (Boorman et al., 1995). These were mapped into four hydrological soil groups (A, B, C, D) to reflect the minimum rate of rainfall infiltration for bare soil after prolonged wetting and the transmission rate within the soil profile, under five land use types; grass, row crops, small grains, semi-naturals and woodlands (Table 3).

Table 3. Pesticide usage and Curve Number (CN) groups for different land use categories.

June Agricultural Census description[1]	**Pesticide usage Group[2]**	**CN group[3]**
Wheat	Cereals	Row crops
Early potatoes	Potatoes	Row crops
Late potatoes	Potatoes	Row crops
Sugar beet	Beet crops	Row crops
Leguminous forage crops	Other fodder crops	Row crops
All Other crops for stockfeeding	Other fodder crops	Row crops
Root crops, brassicas & fodder beet	Vegetable brassicas	Row crops
Winter barley	Cereals	Row crops
Borage	Other arable crops	Row crops
Field beans	Peas & beans	Row crops
Peas for harvesting dry	Peas & beans	Row crops
Maize	Maize & sweetcorn	Row crops
Maize – grain	Maize & sweetcorn	Row crops
Maize – fodder	Maize & sweetcorn	Row crops
Winter oilseed rape	Oilseeds	Row crops
Spring oilseed rape	Oilseeds	Row crops
Linseed	Other arable crops	Row crops
Spring barley	Cereals	Row crops
All Other crops	Other arable crops	Small grains
Bare fallow	Set aside	Semi-natural
Short rotation coppice	Other arable crops	Row crops
Miscanthus	Other arable crops	Row crops
Crops for aromatic or medicinal use	Other arable crops	Row crops
Oats	Cereals	Row crops
Mixed corn	Other arable crops	Small grains
Rye	Other arable crops	Small grains
Triticale	Other arable crops	Small grains

Other peas and beans	Other outdoor vegetables	Row crops
Culinary plants for human consumption (e.g. herbs)	Lettuce & other leafy salads	Row crops
All other veg and salad including carrots and onions	Lettuce & other leafy salads	Row crops
Vining peas for processing	Other outdoor vegetables	Row crops
Orchards commercial	Top fruit & hops	Row crops
Wine grapes	Other soft fruit	Small grains
All other small fruit	Other soft fruit	Small grains
Orchards noncommercial	Top fruit & hops	Row crops
Orchards	Top fruit & hops	Row crops
Strawberries	Strawberries	Small grains
Raspberries	Other soft fruit	Small grains
Blackcurrants	Other soft fruit	Small grains
Temporary Grass	Grassland	Grass
Woodland	Woodland	Woodland
Land used for outdoor pigs	Set aside	Semi-natural
Other non-agricultural land	Set aside	Semi-natural
Permanent Grass	Set aside	Grass
Rough Grazing	Set aside	Semi-natural

[1] The June Survey of Agriculture and Horticulture (JAS) is an annual survey which collects detailed information on arable and horticultural cropping activities, land usage, livestock populations and farming labour force figures - https://data.gov.uk/dataset/june_survey_of_agriculture_and_horticulture_uk
[2] The pesticide usage group reflects the key groups used in surveys reporting publicly available data on pesticide applications (e.g. Garthwaite et al., 2013, 20145, 2015)
[3] Taken from Hess et al. (2010)

The JAS classes were linked to pesticide survey usage categories and, in turn, the CN categories in Hess et al. (2010). Hess et al. (2010) proposed appropriate CNs for each unique combination of grouped soil type and land cover, dependent upon the surface condition which is classified as either ‘good’ or ‘poor’. A CN of 0 represents maximum storage, whilst a score of 100 suggests zero storage (i.e. a totally impermeable soil). The hydrological soil groups reflect the minimum rate of rainfall infiltration for bare soil after prolonged wetting and the transmission rate within the soil profile. Group A soils are characterised by low runoff potential and high infiltration rate even when wetted, with a transmission rate of >7.6 mm/hr. Group B soils have a moderate infiltration rate and are typified by moderate to well drained soils with transmission rates of 3.8 – 7.6 mm/hr. Group C soils have low infiltration rates and are typified by moderately fine to fine texture and a layer impeding downward water movement, yielding transmission rates of 1.3 – 3.8 mm/hr. Finally, group D soils have high runoff potential and very low infiltration rates, typifying clay soils with very low transmission rates of 0 – 1.3 mm/hr. CN values recommended by Hess et al. (2010) are presented in Table 4.

Table 4. Curve Numbers (CN) for surface runoff generation based on Hess et al. (2010).

Hydrological soil group	Vegetation type	Surface condition Good[1]	Poor[2]
A	Grass	39	68
A	Row crops	65	72
A	Small grains	61	65
A	Semi-natural	39	68
A	Woodland	30	45
B	Grass	39	79
B	Row crops	65	81
B	Small grains	61	76
B	Semi-natural	39	79
B	Woodland	30	66
C	Grass	74	86
C	Row crops	82	88
C	Small grains	81	84
C	Semi-natural	74	86
C	Woodland	70	77
D	Grass	80	89
D	Row crops	86	91
D	Small grains	85	88
D	Semi-natural	80	89
D	Woodland	77	83

[1] Good soil structure, limited management activities (e.g. contour ploughing) to reduce runoff transmission from the field

[2]Degraded soil structure resulting in enhanced runoff generation, plus evidence of management activities increasing runoff transmission (e.g. downslope tramlines, compaction due to livestock trampling or use of heavy farm machinery, fine seed beds)

Finally, hydrology outputs from a process-based model developed for national policy support, namely PSYCHIC (Phosphorus and Sediment Yield CHaracterisation In Catchments; Collins et al., 2007; Davison, et al., 2008; Stromqvist et al., 2008; Collins and Anthony, 2008; Collins et al., 2009; Comber et al., 2013; Collins and Zhang, 2016), were used to derive monthly soil runoff partitioning between surface and drain flow pathways for each 1km^2. The PSYCHIC model runs use a combination of baseline climate conditions (1961 to 1990) and 2010 JAS.

3.2.3 Model validation

The validation of a landscape scale model predicting 1km^2 risk surfaces, i.e. providing information to support Tier 1 screening of risk, is inherently difficult.. The model reported here provides information on landscape scale risk and empirical pesticide data, collected at an appropriate resolution, simply does not exist at appropriate scales for validating the modelled patterns of spatial risk. However, previous research (e.g. Stromqvist et al., 2008; Collins and Anthony, 2008; Collins et al., 2016; Collins and Zhang, 2016; Zhang et al., 2017a,b) has evaluated the catchment and broader scale spatial patterns predicted for aggregated diffuse pollution (nutrients and sediment, not pesticides) delivery to watercourses using the underlying algorithms from PSYCHIC that are incorporated in the landscape model, using available local (i.e. original PSYCHIC model research project) or strategic monitoring data in the form of 1991-2010 PARCOM (Neal and Davies, 2003) reporting and the Harmonized Monitoring Scheme (https://data.gov.uk/dataset/b17a2efa-bdd6-4740-8030-fb87f7f2bcff/historic-uk-water-quality-sampling-harmonised-monitoring-scheme-detailed-data) at 33 stations for the period 1980-2010. Paris Commission (PARCOM) monitoring is undertaken as part of the 1992 OSPAR (Oslo–Paris) Convention which combined the 1972 Oslo Convention on dumping waste at sea and the 1974 Paris Convention on land-based sources of marine pollution. PARCOM monitoring is undertaken to report the delivery of terrestrial pollutants to the maritime area in accordance with the OSPAR Convention. The Harmonized Monitoring Scheme is a long-term water quality scheme in the UK that was initiated by the Department of the Environment in 1974.

4. Results

The field and catchment scale models were coded in R and interactive web tools with an Open Street Map front end were created in RMarkdown using the *leaflet*, *flexdashboard*, *shiny*, *sp*, *dygraphs* and *reshape2* R packages. Recent and short-term forecast rainfall was recognised as a critical input for each scale in order to determine field runoff and field-to-channel delivery risk. For each study catchment, live weather data and precipitation forecasts from the Meteorological Office (the UK’s national weather service) *DataPoint* API (Met Office, 2018) were downloaded for each day, interpolated into a 1 km^2 grid and stored in raster stack. These were used to serve the online models with antecedent, current and predicted rainfall data for each 1 km^2. The online web tools are dynamic, calculating field runoff or field-to-channel delivery risk at each location from the live precipitation data and the user inputs. A zoomable OpenStreetMap layer provided the background mapping.

4.1 Field scale tool

The intention of the field scale tool was that it would be used by farmers and farm managers to inform their day-to-day decision making around agricultural chemical applications. The web interface asks users to enter a postcode, and then to click on an individual 1 km^2 grid cell. For the purposes of the models demonstrated here, the interface in Wales assumes an Acid herbicide application decision and in the East of England a Metaldehyde application (only the Wales tool is illustrated). The runoff risk for the selected grid cell for the next 5 days is shown in text format below the map and there are a number of tabs containing additional information. A screen grab of the catchment scale tool is shown in Figure 3. Here rainfall and runoff risk are not quantified, they are simply stated if predicted to be present at the selected location for the selected time period +5 days, as described above.

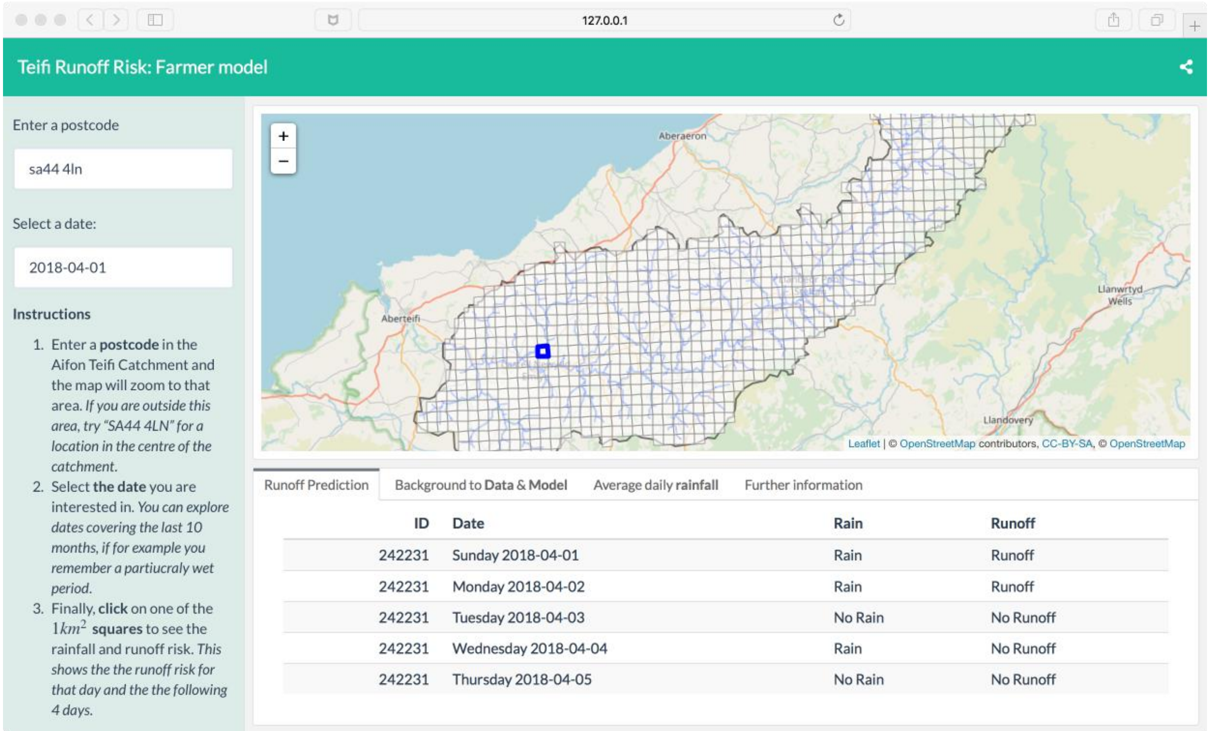

Figure 3. A screenshot of output from the Teifi catchment field scale runoff risk model at https://saric.shinyapps.io/tei_field/.

4.2 Catchment scale tool

The catchment scale tool was aimed at land and environmental managers with catchment / sub-catchment and watershed remits, including local water companies. Runoff and pesticide field-to-channel delivery risk is mapped and indicates locations with varying risk, given current and antecedent rainfall conditions, with the aim of supporting drinking water abstraction operations. The on-line tool asks users to indicate the agro-chemical they are interested in, the status of the soil and the date for which they require field-to-channel delivery risk estimates. For this proof of concept tool, the choices for agro-chemicals are limited to "Metaldehyde" and "Acid Herbicide", and the choices for soil status to "Good" or "Poor". The runoff risk is *R* (mm) from Equation 15 was categorised into 4 classes of risk: *None* when R = 0, *Low* when 0 < R <= 0.02, *Moderate* when 0.02 < R <= 0.05 and *High* when R > 0.05. In contrast to the field scale tool, the aim here was to provide users with landscape and catchment scale policy responsibilities with some information about the degree of pesticide delivery risk across the 1 km^2 grid cells comprising the study area. The user can pick any date between current date and October 2017 with the aim of allowing users to explore known runoff events and the degree to which the tool predicted any locally observed runoff and this is supported by an interactive (dy)graph of the mean rainfall in this period for this area. When the user selects a date, the current and previous 5-day rainfall for each 1 km^2 are extracted and the model is run generating a surface of predicted pesticide delivery risk. The boxplots show the rainfall for the previous 5 days and the date being queried. A screen grab of the catchment scale model application to the Wissey catchment is shown in Figure 4.

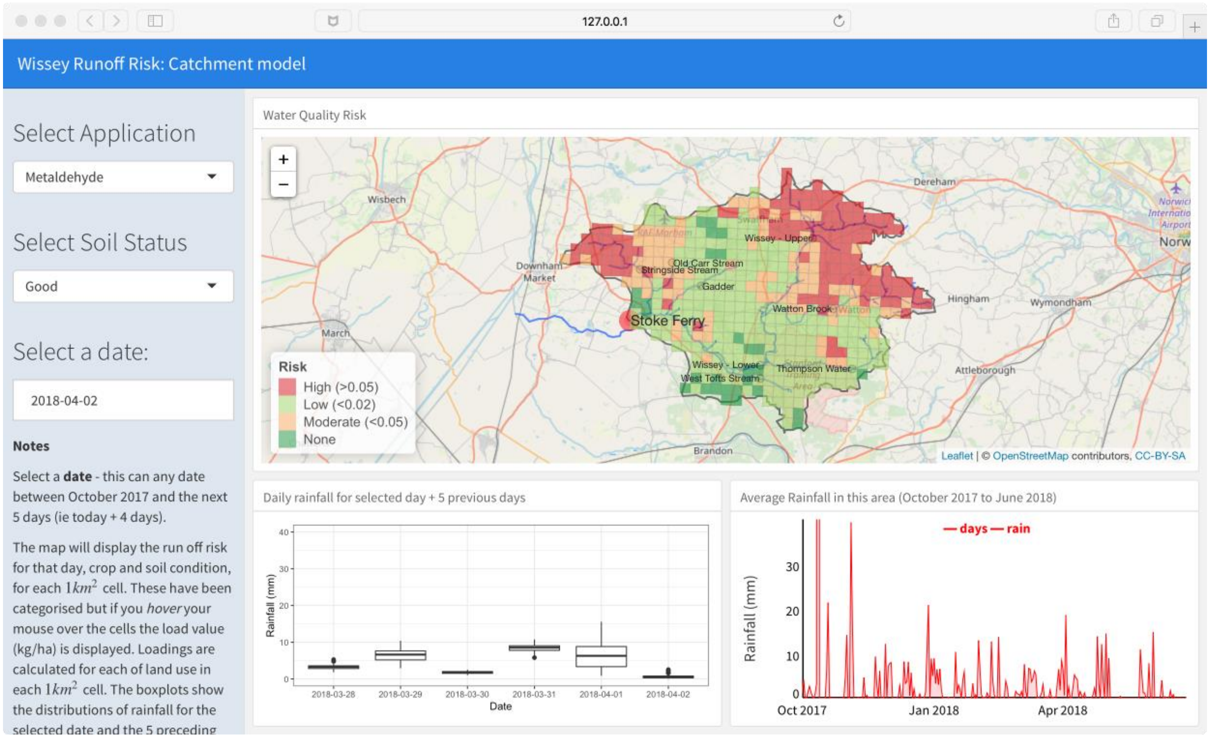

Figure 4. A screenshot of output from the Wissey catchment scale field-to-channel delivery risk model at https://saric.shinyapps.io/wis_catch/.

5. Concluding Remarks

The effective use of agrochemicals in modern agriculture contributes to sustained crop yields and quality. However, agrochemicals are less effective when they ‘run off’ into surface and groundwaters soon after they are applied. The risk of this happening increases when agrochemicals are applied to wet (saturated) soils and when rainfall occurs soon after application. Runoff and associated pollutant delivery from field-to-channel also has negative impacts on environmental and drinking water quality when agrochemicals are transferred to surface or groundwater.

This paper describes a novel, generic and parsimonious modelling framework that integrates dual-scale soil water interaction models with real-time weather data. It addresses a number of impediments to the use of existing runoff risk models to inform on-farm management decisions and catchment management.
i) Most soil-water interaction models have high data and input parameter requirements to generate daily time-step simulations of processes related plant and crop growth.
ii) Consequently they require in-depth knowledge about input process parameters.
iii) They frequently require data which may not be available, for example to non-academic or non-research organisations, or to farmers and commercial companies.
iv) Many of these models perform poorly when compared with observed monitoring data (e.g. Zeiger and Hubbart, 2016).
v) Finally, because of these issues, existing models are not easily integrated into tools able to quantify the real-time field runoff and field-to-channel delivery risks which are required to support more reactive and effective agrochemical management decisions on the ground.

The dynamic, real-time decision tools developed in this research do not address all of these issues (there remain difficulties in validating the detailed spatial patterns predicted by any catchment scale model, for example). However, the provision of spatially- and temporally-explicit runoff and pesticide delivery risk information using parsimonious models is novel. We have demonstrated their applicability for two spatial scales of decision making: on-farm and catchment. The individual components of the parsimonious tools are not new: field and catchment scale models of pesticide and herbicide runoff have existed for a long time. But, critically, existing tools fail to provide *timely* and thereby *useful* information to managers. There are many live and location specific weather forecasting websites, smartphone apps and tools. As yet, however, real-time forecasting and soil water models have not been linked in an accessible and user-friendly way. In most decision tools, the model data inputs are relatively static (e.g. cropping systems, soil conditions, measures of catchment scale field drainage, etc) and do not support location- and time-specific queries. The result is that the modelled soil-water interactions and pesticide persistence represent some kind of generalised overall runoff trend rather than a specific local runoff measure.

There are a number of areas of potential future work emerging from this research for the further development of this modelling framework. The field and catchment scale models are very much proofs of concept and demonstrate how parsimonious but sensitive runoff risk models could be included in such frameworks. The utility of the tools and the interfaces from the end user perspective could be enhanced and the scope of the tools could be expanded in a number of ways. In our generic approach for both field and catchment scales, the critical variables driving field runoff and field-to-channel delivery risk are those related to antecedent, current and forecast rainfall in combination with fundamental intrinsic controls. In previous models, these have been assumed under a suite of potential scenarios that the user has to choose from. However, the ability to link to spatially- and temporally- explicit data for the rainfall variables through APIs offers a new avenue for enhancing the wider application and utility of soil-water-connectivity models. The future ability to serve many different types of geo-spatial data in this way via distributed data portals will only increase, reducing the dependency on locally held data. The landscape scale tool could be expanded to include nested watershed, catchment and sub-catchment scales and any corresponding aggregation associated with instream transfer processes. A further area for development would be to account for "noise" in runoff from agricultural applications, not least of which are point pollution due to poor on farm practice (incidental spillages, etc), runoff from domestic and managed green space applications as well as pesticide spray drift. A final and critical area of further work in the context of the approaches described is the inclusion of high accuracy rainfall data. This project used publicly available rainfall data served through the UK Met Office's API and interpolated over a 1km^2 grid. Higher quality data is not provided for free. As the models inherently depend on rainfall (to parameterise the soil wetness factors through antecedent rainfall, to model current risk and determine future risk projections), the greatest influence on the quality of the model outputs is driven by this data.

In summary, the tools developed in this research provide user interfaces to stripped down, parsimonious soil-water-connectivity models that take advantage of the availability of live rainfall data. Their components reflect the importance of knowledge of past and current rainfall as drivers of field runoff and field-to-channel delivery. To this end, each model pre-computed long-term water content for different soil types and crops, was linked to a live rainfall data feed and requested a very small amount of information from users (date, soil status, crop type) from which field runoff and field-to-channel delivery risk was computed using antecedent and current rainfall. The wider applicability of this research is underpinned by the generic nature of the parsimonious modelling framework. Assuming the availability of relevant mechanistic understanding and information on application doses, the models could easily be extended to predict risks to water quality and the wider environment for ***any*** agricultural application at the farm decision scale or at the landscape management scale. Future work will develop a more strategic and commercial framework for a wider suite of parsimonious models.

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